

Energy spectrum of a harmonically trapped two-atom system with spin-orbit coupling

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Ultracold atomic gases provide a novel platform with which to study spin-orbit coupling, a mechanism that plays a central role in the nuclear shell model, atomic fine structure and two-dimensional electron gases. This paper introduces a theoretical framework that allows for the efficient determination of the eigenenergies and eigenstates of a harmonically trapped two-atom system with short-range interaction subject to an equal mixture of Rashba and Dresselhaus spin-orbit coupling created through Raman coupling of atomic hyperfine states. Energy spectra for experimentally relevant parameter combinations are presented and future extensions of the approach are discussed.

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Over the past decade, much progress has been made in preparing isolated ultracold few-atom systems experimentally [1–4]. Moreover, a variety of tools for manipulating and probing such systems have been developed. On the theoretical side, a number of analytical and numerical approaches have been developed [5–13]. A large number of analytical treatments approximate the true alkali atom-alkali atom potential by a zero-range potential [8, 14–16]. This replacement yields reliable results in the low-energy regime where the de Broglie wave length is larger than the van der Waals length. For example, using zero-range contact interactions, the energy spectrum of two harmonically trapped atoms has been determined analytically [8–10]. These two-body solutions are available in 1D, 2D and 3D [8], and have played a vital role in guiding and interpreting experiments [17–19] as well as in theoretical studies of the two-body dynamics [20, 21] and of larger harmonically trapped systems [11–13, 22–24].

Recently, synthetic gauge fields, which allow for the realization of Hamiltonians that contain spin-orbit coupling terms, have been realized experimentally [25–35]. The purpose of this paper is to address how the trapped two-particle spectrum, obtained by modeling the two-body interaction via a zero-range δ -function, changes in the presence of spin-orbit and Raman coupling. While the two-particle system with spin-orbit coupling in free space [36–39] as well as the trapped single-particle system with spin-orbit coupling [40, 41] have received considerable attention, little is known about the trapped two-particle system with spin-orbit coupling and two-body interaction [42, 43]. In going from the trapped single-atom to the trapped two-atom system, a new length scale, i.e., the atom-atom scattering length, comes into play. Thus, an interesting question concerns the interplay between the interaction energy and the energy scales associated with the spin-orbit and Raman coupling strengths.

Our framework applies to the situation where the spin-orbit (or more precisely, spin-momentum) coupling term acts, as in recent experiments [29–35], along one spatial direction, say the x -direction. This corresponds to an equal mixture of Rashba and Dresselhaus spin-orbit coupling [44, 45]. For simplicity, we assume that the harmonic confinement in the other two spatial directions is

much larger than that in the direction where the spin-orbit coupling term acts. This assumption reduces the problem to an effective one-dimensional Hamiltonian in the x -coordinates with effective 1D two-body interaction. The relationship between the true 3D atom-atom and effective 1D atom-atom interaction has been derived in Refs. [46–48]. We find analytical solutions to the two-atom system for arbitrary spin-orbit coupling strength and scattering length and vanishing Raman coupling strength. The case of non-zero Raman coupling strength is treated by expanding the system Hamiltonian in terms of the eigenstates for vanishing Raman coupling strength. We find that the relevant Hamiltonian matrix elements have closed analytical expressions, leaving the matrix diagonalization as the only numerical step. The developed framework can, as discussed toward the end of our paper, be readily generalized to a spherically-symmetric harmonic trap or an axisymmetric trap. Moreover, the framework developed also lays the groundwork for treating dynamical aspects of trapped two-body systems with non-vanishing spin-orbit and Raman coupling strengths and for treating the corresponding three-body system.

We consider two structureless one-dimensional particles of mass m subject to a single-particle spin-orbit coupling term of strength k_{so} , a Raman coupling term with strength Ω , detuning δ , and an external harmonic potential with angular trapping frequency ω . For $k_{\text{so}} = \Omega = \delta = 0$, the two-particle Hamiltonian is given by H_{sr} ,

$$H_{\text{sr}} = \sum_{j=1}^2 \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \frac{1}{2} m \omega^2 x_j^2 \right) + V_{2b}(x_1 - x_2), \quad (1)$$

where x_j denotes the position coordinate of the j th particle and V_{2b} the short-range interaction potential. For non-zero k_{so} , Ω and δ , the two-particle Hamiltonian is given by H ,

$$H = H_{\text{sr}} \hat{I} + \sum_{j=1}^2 \left[\frac{\hbar k_{\text{so}}}{m} p_{xj} \sigma_y^{(j)} + \frac{\Omega}{2} \sigma_x^{(j)} + \frac{\delta}{2} \sigma_y^{(j)} \right], \quad (2)$$

where $\sigma_x^{(j)}$ and $\sigma_y^{(j)}$ denote Pauli matrices, \hat{I} the identity matrix and p_{xj} the momentum of the j th particle.

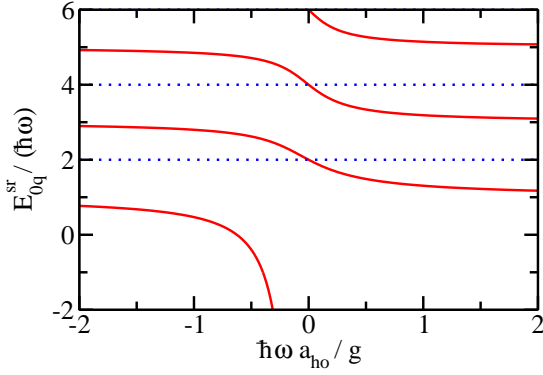


FIG. 1: (Color online) Zero-range energies E_{0q}^{sr} as a function of $\hbar\omega a_{ho}/g$. Solid and dotted lines show the energies corresponding to states that are even and odd, respectively, in the relative coordinate.

In the following, we first derive solutions to the time-independent Schrödinger equation governed by H with $\Omega = 0$ and then discuss how to obtain the solutions for non-zero Ω .

To determine the eigenstates and eigenenergies of H , we perform a rotation in spin space [49]. Specifically, we define \tilde{H} via a unitary transformation of H , $\tilde{H} = U^\dagger H U$, where $U = \exp[\imath(\sigma_x^{(1)} + \sigma_x^{(2)})\pi/4]$. The eigenenergies of the Hamiltonian H and \tilde{H} coincide while the eigenstates Ψ of the Hamiltonian H are related to the eigenstates $\tilde{\Psi}$ of the Hamiltonian \tilde{H} through $\Psi = U\tilde{\Psi}$. A straightforward calculation shows that $U^\dagger \sigma_q^{(j)} U = \sigma_x^{(j)}$ and $\sigma_z^{(j)}$ for $q = x$ and y , respectively. Correspondingly, we have

$$\tilde{H} = H_{sr}\hat{I} + \sum_{j=1}^2 \left[\frac{\hbar k_{so}}{m} p_{xj} \sigma_z^{(j)} + \frac{\Omega}{2} \sigma_x^{(j)} + \frac{\delta}{2} \sigma_z^{(j)} \right]. \quad (3)$$

For $\Omega = 0$, \tilde{H} is diagonal in the pseudo-spin basis $|\uparrow\rangle_1 |\uparrow\rangle_2$, $|\uparrow\rangle_1 |\downarrow\rangle_2$, $|\downarrow\rangle_1 |\uparrow\rangle_2$ and $|\downarrow\rangle_1 |\downarrow\rangle_2$ with diagonal elements $\tilde{H}^{\uparrow\uparrow}$, $\tilde{H}^{\uparrow\downarrow}$, $\tilde{H}^{\downarrow\uparrow}$ and $\tilde{H}^{\downarrow\downarrow}$. To find the corresponding eigenstates, we approximate the two-body interaction by a delta-function interaction with coupling constant g , $V_{2b}(x_1 - x_2) = g\delta(x_1 - x_2)$. For this interaction model, the eigenenergies and eigenstates of H_{sr} are known in compact form [8]. States that are even in the relative coordinate are affected by the coupling constant g while those that are odd in the relative coordinate are not. For states that are even in the relative coordinate, the eigenenergies E_{nq}^{sr} of H_{sr} (see solid lines in Fig. 1 for the $n = 0$ energies) are given by $(n + 2q + 1)\hbar\omega$, where the center of mass quantum number n takes the values $n = 0, 1, \dots$ and the non-integer quantum number q is determined by the transcendental equation [8]

$$\frac{2\Gamma(-q + 1/2)}{\Gamma(-q)} = -\frac{g}{\sqrt{2}\hbar\omega a_{ho}}; \quad (4)$$

here, a_{ho} denotes the harmonic oscillator length, $a_{ho} = \sqrt{\hbar/(m\omega)}$. The corresponding eigenfunctions $\psi_{nq}^{sr}(x, X)$ are given by $\phi_q(x)\Phi_n(X)$, where the relative and center of mass coordinates are defined through $x = (x_1 - x_2)/\sqrt{2}$ and $X = (x_1 + x_2)/\sqrt{2}$, respectively. The relative wave functions $\phi_q(x)$ can be written in terms of the confluent hypergeometric function U [8], $\phi_q(x) = N_q U(-q, 1/2, (x/a_{ho})^2) \exp[-x^2/(2a_{ho}^2)]$, where N_q denotes a normalization constant. The center of mass functions $\Phi_n(X)$ are given by the one-dimensional harmonic oscillator functions for a mass m particle, $\Phi_n(X) = N_n^{ni} H_n(X/a_{ho}) \exp[-X^2/(2a_{ho}^2)]$, where H_n denotes the Hermite polynomial of order n and $N_n^{ni} = (\sqrt{\pi}2^n n! a_{ho})^{-1/2}$. For states that are odd in the relative coordinate, the eigenenergies E_{nq}^{sr} of H_{sr} (see dotted lines in Fig. 1 for the $n = 0$ energies) are given by $(n + 2q + 2)\hbar\omega$, where q and n take the values $0, 1, \dots$. In this case, the eigenfunctions $\psi_{nq}^{sr}(x, X)$ are simply products of the non-interacting harmonic oscillator functions in x and X .

In addition to using the known properties of H_{sr} , we take advantage of the fact that the kinetic energy $(p_{x1}^2 + p_{x2}^2)/(2m)$ of H_{sr} and the k_{so} dependent terms can be combined,

$$\frac{p_{xj}^2}{2m} \pm \frac{\hbar k_{so}}{m} p_{xj} = \frac{(p_{xj} \pm \hbar k_{so})^2}{2m} - \frac{\hbar^2 k_{so}^2}{2m}. \quad (5)$$

This identity suggests that the momentum-dependent spin-orbit coupling terms add a “momentum boost” to the solutions $\psi_{nq}^{sr}(x, X)$ of H_{sr} . Indeed, it is readily verified that the eigenstates of $\tilde{H}^{\uparrow\uparrow}$, $\tilde{H}^{\uparrow\downarrow}$, $\tilde{H}^{\downarrow\uparrow}$, and $\tilde{H}^{\downarrow\downarrow}$ are given by

$$\tilde{\psi}_{nq}^{\uparrow\uparrow}(x, X) = \exp(-\imath\sqrt{2}k_{so}X)\psi_{nq}^{sr}(x, X), \quad (6)$$

$$\tilde{\psi}_{nq}^{\uparrow\downarrow}(x, X) = \exp(-\imath\sqrt{2}k_{so}x)\psi_{nq}^{sr}(x, X), \quad (7)$$

$$\tilde{\psi}_{nq}^{\downarrow\uparrow}(x, X) = \exp(\imath\sqrt{2}k_{so}x)\psi_{nq}^{sr}(x, X), \quad (8)$$

and

$$\tilde{\psi}_{nq}^{\downarrow\downarrow}(x, X) = \exp(\imath\sqrt{2}k_{so}X)\psi_{nq}^{sr}(x, X), \quad (9)$$

respectively. For fixed g and n and vanishing δ , the states given in Eqs. (6)-(9) are degenerate with eigenenergies $E_{nq} = E_{nq}^{sr} - \hbar^2 k_{so}^2/m$. For $|g| = \infty$, the degeneracy doubles (see the crossings of the solid and dotted lines in Fig. 1) since q takes the values $1/2, 3/2, \dots$ for ψ_{nq}^{sr} that are even in x and the values $0, 1, 2, \dots$ for ψ_{nq}^{sr} that are odd in x , i.e., since each of the ψ_{nq}^{sr} odd in x is degenerate with one of the ψ_{nq}^{sr} even in x . For non-vanishing δ , the energies are shifted by $\delta, 0, 0$ and $-\delta$, respectively. The eigenenergies are simply the sum of a term that depends on the coupling constant g , a center of mass contribution that is characterized by n , a term that depends on the square of the spin-orbit coupling strength k_{so} and a term that depends on the detuning δ .

If Ω is non-zero, the Hamiltonian \tilde{H} expressed in the $|\uparrow\rangle_1|\uparrow\rangle_2, |\uparrow\rangle_1|\downarrow\rangle_2, |\downarrow\rangle_1|\uparrow\rangle_2, \text{ and } |\downarrow\rangle_1|\downarrow\rangle_2$ pseudo-spin basis is no longer diagonal. To determine the eigenenergies and eigenstates for non-zero Ω , we expand \tilde{H} in terms of the eigenstates $\tilde{\psi}_{nq}^{\sigma'_1\sigma'_2}$, where σ_1 and σ_2 take the values \uparrow and \downarrow . The off-diagonal matrix elements $H_{n'q',nq}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$,

$$H_{n'q',nq}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} = \frac{\Omega}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\tilde{\psi}_{n'q'}^{\sigma'_1\sigma'_2})^* \tilde{\psi}_{nq}^{\sigma_1\sigma_2} dx dX, \quad (10)$$

can be separated into two one-dimensional integrals,

$$H_{n'q',nq}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} = \frac{\Omega}{2} I_{q'q}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} J_{n'n}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}, \quad (11)$$

where

$$I_{q'q}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} = \int_{-\infty}^{\infty} \exp(\eta i \sqrt{2} k_{\text{so}} x) [\phi_{q'}(x)]^* \phi_q(x) dx \quad (12)$$

and

$$J_{n'n}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} = \int_{-\infty}^{\infty} \exp(\xi i \sqrt{2} k_{\text{so}} X) [\Phi_{n'}(X)]^* \Phi_n(X) dX \quad (13)$$

The sign of the exponent is determined by the pseudo-spin combinations: $(\eta, \xi) = (-, +), (+, +), (-, -)$ and $(+, -)$ for $(\sigma'_1\sigma'_2, \sigma_1\sigma_2) = (\uparrow\uparrow, \uparrow\downarrow), (\uparrow\uparrow, \uparrow\uparrow), (\downarrow\downarrow, \uparrow\downarrow)$ and $(\downarrow\downarrow, \uparrow\uparrow)$, respectively.

The integral $J_{n'n}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$ over the center of mass coordinate coincides with the Fourier transform of the product of two one-dimensional harmonic oscillator eigenstates. For $\xi = \pm$ ($n' \leq n$), we find [50]

$$J_{n'n}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2} = a_{\text{ho}} \sqrt{\pi} N_{n'}^{\text{ni}} N_n^{\text{ni}} n'! 2^{(n+n')/2} \times L_{n'}^{(n-n')} ((a_{\text{ho}} k_{\text{so}})^2) (\pm i k_{\text{so}} a_{\text{ho}})^{n-n'} \exp[-(k_{\text{so}} a_{\text{ho}})^2 / 2], \quad (14)$$

where $L_n^{(n-n')}$ denotes the associated Laguerre polynomial.

The integral $I_{q'q}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$ over the relative coordinate can be performed by expanding $[\phi_{q'}(x)]^*$ and $\phi_q(x)$ in

terms of the non-interacting harmonic oscillator functions $\phi_l^{\text{ni}}(x)$, $\phi_q(x) = \lim_{l_{\text{max}} \rightarrow \infty} \sum_{l=0}^{l_{\text{max}}} c_l^{(q)} \phi_l^{\text{ni}}(x)$, where the expansion coefficients $c_l^{(q)}$ can be obtained analytically [8]. The integral $I_{q'q}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$ then becomes a double sum over integrals that have the same structure as the center of mass integrals $J_{n'n}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$. In the calculations reported below, we use a finite cutoff l_{max} . The “optimal” cutoff depends on the value of g considered, the number of relative functions $\phi_q(x)$ included in the basis and the desired accuracy. For $|g| = \infty$, we find, as in the $g = 0$ case, a closed analytical expression for the integral $I_{q'q}^{\sigma'_1\sigma'_2,\sigma_1\sigma_2}$. Having analytical expressions for the matrix elements of \tilde{H} , the eigenenergies can be obtained through matrix diagonalization.

To obtain basis functions with good quantum numbers, we work with linear combinations of the functions given in Eqs. (6)-(9), i.e., we work with the basis functions $\tilde{\psi}_{X,\pm} = (\tilde{\psi}_{nq}^{\uparrow\uparrow} |\uparrow\rangle_1 |\uparrow\rangle_2 \pm \tilde{\psi}_{nq}^{\downarrow\downarrow} |\downarrow\rangle_1 |\downarrow\rangle_2) / \sqrt{2}$ and $\tilde{\psi}_{x,\pm} = (\tilde{\psi}_{nq}^{\uparrow\downarrow} |\uparrow\rangle_1 |\downarrow\rangle_2 \pm \tilde{\psi}_{nq}^{\downarrow\uparrow} |\downarrow\rangle_1 |\uparrow\rangle_2) / \sqrt{2}$. By properly combining the parts of $\tilde{\psi}_{nq}^{\text{sr}}$ that are even or odd in the relative coordinate and even or odd in the center of mass coordinate, we construct basis functions that are eigenstates of the operators P_{12} and Y_{12} . The operator P_{12} exchanges the coordinates (position and spin) of particles 1 and 2. Basis functions that are unchanged under the operation P_{12} are needed to describe states with bosonic symmetry ($p_{12} = +1$) and those that pick up a minus sign under the operation P_{12} are needed to describe states with fermionic symmetry ($p_{12} = -1$). The operator Y_{12} can be written as $\sigma_x^{(1)} \sigma_x^{(2)} P P_{12}$, where the parity operator P changes x_j to $-x_j$ ($j = 1$ and 2). The Y_{12} operator determines the “helicity” of the system. We label the eigenstates by (p_{12}, y_{12}) , where $p_{12} = \pm 1$ and $y_{12} = \pm 1$ are defined by their actions on an eigenstate. The basis functions with $(+1, +1)$ symmetry, for example, are given by $\tilde{\psi}_{X,+}$ with $\phi_q(x)$ even and $\Phi_n(X)$ even, by $\tilde{\psi}_{X,-}$ with $\phi_q(x)$ even and $\Phi_n(X)$ odd, by $\tilde{\psi}_{x,+}$ with $\phi_q(x)$ even and $\Phi_n(X)$ even, and by $\tilde{\psi}_{x,-}$ with $\phi_q(x)$ odd and $\Phi_n(X)$ even.

As an example, Figs. 2(a)-2(c) show energy spectra corresponding to eigenstates with $(p_{12}, y_{12}) = (+1, +1)$ as a function of the Raman coupling strength Ω for vanishing detuning δ , small coupling constant g , $g \approx 0.1414 a_{\text{ho}} \hbar \omega$, and three different spin-orbit coupling strengths k_{so} . The energy spectrum in Fig. 2(a) is, to leading order, given by the spectrum for $\delta = k_{\text{so}} = g = 0$. In this limiting case, the energies are equal to $(2j+1)\hbar\omega \pm \Omega$ and $2j\hbar\omega$, where $j = 0, 1, \dots$. Finite g and k_{so} values introduce shifts and avoided crossings. Specifically, the small positive coupling constant g introduces a positive energy shift for the states that are even

in the relative coordinate, which—in first-order perturbation theory—is given by $\frac{1}{\sqrt{2\pi}} \frac{(2q)!}{(q!)^2 4^q} g / a_{\text{ho}}$. The spin-orbit coupling term introduces, in the small Ω regime, a small down shift that is proportional to k_{so}^2 . This down shift is negligible in Fig. 2(a) but clearly visible in Figs. 2(b) and 2(c). Moreover, the spin-orbit coupling introduces avoided crossings. The broadest avoided crossings occur around $\Omega = \hbar\omega$, where states with the same q but n quantum numbers that differ by one are coupled. The reason is that the spin-orbit coupling term connects, via the total momentum operator, states in first-order perturbation theory if the states' n quantum numbers differ

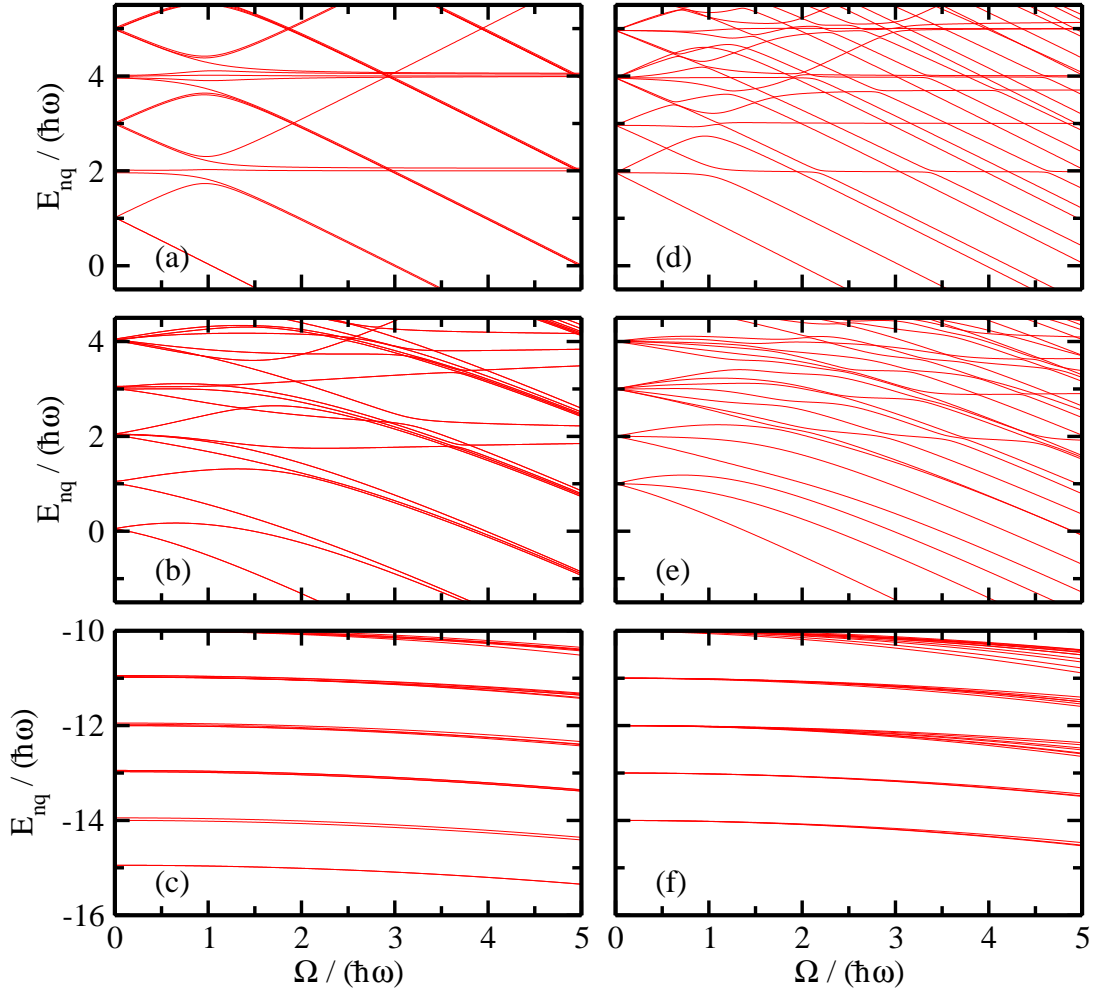


FIG. 2: (Color online) Eigenenergies E_{nq} corresponding to eigenstates with $(p_{12}, y_{12}) = (+1, +1)$ as a function of Ω for $\delta = 0$, and (a) $a_{\text{ho}}k_{\text{so}} = 0.2$ and $g = a_{\text{ho}}\hbar\omega/\sqrt{50}$; (b) $a_{\text{ho}}k_{\text{so}} = 1$ and $g = a_{\text{ho}}\hbar\omega/\sqrt{50}$; (c) $a_{\text{ho}}k_{\text{so}} = 4$ and $g = a_{\text{ho}}\hbar\omega/\sqrt{50}$; (d) $a_{\text{ho}}k_{\text{so}} = 0.2$ and $|g| = \infty$; (e) $a_{\text{ho}}k_{\text{so}} = 1$ and $|g| = \infty$; and (f) $a_{\text{ho}}k_{\text{so}} = 4$ and $|g| = \infty$, respectively.

by one and in higher-order perturbation theory otherwise.

Figures 2(d)-2(f) show energy spectra for the strong coupling limit, i.e., for $|g| \rightarrow \infty$, as a function of the Raman coupling Ω for vanishing detuning δ . To facilitate the comparison between the large and small g limits, the spin-orbit coupling strengths k_{so} in Figs. 2(d)-2(f) are the same as in Figs. 2(a)-2(c). In the regime where $\Omega \ll \hbar^2 k_{\text{so}}^2/m$, the energies change approximately linearly with Ω (with positive, vanishing or negative slope). When $\Omega \gg \hbar^2 k_{\text{so}}^2/m$, the low-lying portion of the energy spectrum consists of approximately parallel energy levels that can be parameterized as $c - \Omega$, where c is a constant.

As already aluded to in the introduction, the theoretical framework developed can be generalized to higher-dimensional trapping geometries. For a spherically symmetric 3D system, e.g., the eigenstates of the 3D Hamiltonian H_{sr} with 3D contact interaction can be expanded in terms of products of 2D and 1D harmonic oscillator

states using cylindrical coordinates. As in the 1D case pursued in this work, the matrix elements for the higher-dimensional system can be calculated analytically. Axisymmetric harmonic traps with spin-orbit coupling in one direction can be treated analogously. Furthermore, using the eigenstates of the trapped three-particle system in 1D, 2D or 3D with contact interactions [11, 22, 23] and expressing the three-particle Hamiltonian in terms of the eight pseudo-spin states, a non-zero Ω introduces off-diagonal elements that can be calculated analytically following steps similar to those discussed in this paper.

Summarizing, this work introduced a theoretical framework that allows for the efficient determination of the energy spectrum and eigenstates of the trapped two-particle system in 1D with contact interaction and spin-orbit and Raman coupling terms. The energy spectra show a rich dependence on the interaction, spin-orbit and Raman coupling strengths. The framework presented provides an important stepping stone for treating

more complicated systems with spin-orbit coupling, such as higher-dimensional two-body systems and three-body systems.

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